

1-12 3-13 5-19 normalized bonds: 5-10 5-6 6-7 7-8 8-9 9-10 15-16 15-20 16-17 17-18 18-19 19-20 isolated ring systems: containing 15:

G2:0,S,N,CH3,Et,n-Pr,MeO,EtO,n-PrO

Match level: 1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:CLASS 13:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom chain nodes : 10 11 12 13 14 24 25 ring nodes : 1 2 3 4 5 6 7 8 9 15 16 17 18 19 20 chain bonds : 6-10 10-11 10-24 11-12 11-13 12-14 12-25 14-15 ring bonds : 1-2 1-6 2-3 3-4 3-7 4-5 4-8 5-6 7-9 8-9 15-16 15-20 16-17 17-18 18-19 19-20 exact/norm bonds : 3-4 3-7 4-5 4-8 6-10 7-9 8-9 10-11 10-24 11-12 11-13 12-14 12-25 14-15 normalized bonds : 1-2 1-6 2-3 5-6 15-16 15-20 16-17 17-18 18-19 19-20 isolated ring systems : containing 1 : 15 : G1:C,O Match level : 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 24:CLASS 25:CLASS Generic attributes : 14: Saturation : Unsaturated Number of Carbon Atoms : less than 7 Number of Hetero Atoms : Exactly 1

C:\Program Files\Stnexp\Queries\rkc446b.str

C:\Program Files\Stnexp\Queries\rkc446n.str

chain nodes:
1 2 3 4 5 13 14 16
ring nodes:
6 7 8 9 10 11
chain bonds:
1-13 1-2 1-16 2-3 2-4 3-5 3-14 5-6
ring bonds:
6-11 6-7 7-8 8-9 9-10 10-11
exact/norm bonds:

exact/norm bonds : 1-2 1-16 2-3 2-4 3-5 5-6 exact bonds :

1-13 3-14 normalized bonds :

6-11 6-7 7-8 8-9 9-10 10-11

G1:C,O

G2:O,S,N,CH3,Et,n-Pr,MeO,EtO,n-PrO

Match level: 1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom

13:CLASS 14:CLASS 16:Atom Generic attributes : 5:

Saturation : Unsaturated Number of Hetero Atoms : Exactly 1

C:\Program Files\Stnexp\Queries\rkc446.str chain nodes : 10 11 12 13 14 24 25 27 ring nodes : 1 2 3 4 5 6 7 8 9 15 16 17 18 19 20 chain bonds : 6-10 10-11 10-24 11-12 11-13 12-14 12-25 14-15 ring bonds : 1-2 1-6 2-3 3-4 3-7 4-5 4-8 5-6 7-9 8-9 15-16 15-20 16-17 17-18 18-19 19-20 exact/norm bonds : 3-4 3-7 4-5 4-8 6-10 7-9 8-9 10-11 10-24 11-12 11-13 12-14 12-25 14-15 normalized bonds : 1-2 1-6 2-3 5-6 15-16 15-20 16-17 17-18 18-19 19-20 isolated ring systems : containing 1 : 15 : G1:C,O

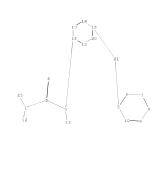
Match level :

1.Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 24:CLASS 25:CLASS 27:CLASS 28:CLASS 26:CLASS 2 Generic attributes : 14:

Saturation : Unsaturated Number of Carbon Atoms : less than 7 Number of Hetero Atoms : Exactly 1

C:\Program Files\Stnexp\Queries\rkc446j.str





```
1 2 3 4 12 13 21 23
ring nodes:
5 6 7 8 9 10 15 16 17 18 19 20
chain bonds:
1-12 1-2 1-23 2-3 2-4 3-13 3-16 5-21 19-21
ring bonds:
5-10 5-6 6-7 7-8 8-9 9-10 15-16 15-20 16-17 17-18 18-19 19-20
exact/norm bonds:
1-2 1-23 2-3 2-4 3-16 5-21 19-21
exact bonds:
1-12 3-13
normalized bonds:
5-10 5-6 6-7 7-8 8-9 9-10 15-16 15-20 16-17 17-18 18-19 19-20
exact bond:
1-12 3-13
normalized bonds:
5-10 5-6 6-7 7-8 8-9 9-10 15-16 15-20 16-17 17-18 18-19 19-20
isolated ring systems:
```

G1:C,O

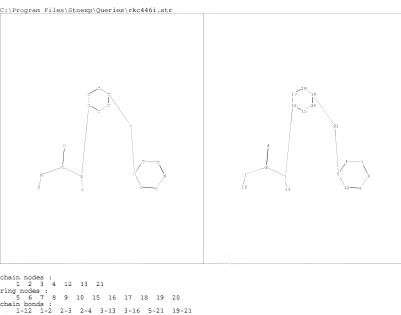
chain nodes :

G2:O,S,N,CH3,Et,n-Pr,MeO,EtO,n-PrO

containing 15 :

Match level: 1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:CLASS 13:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS 23:Atom Generic attributes:

23: Number of Carbon Atoms : 7 or more Type of Ring System : Polycyclic



ring bonds:
5-10 5-6 6-7 7-8 8-9 9-10 15-16 15-20 16-17 17-18 18-19 19-20 exact/norm bonds:
1-2 2-3 2-4 3-16 5-21 19-21 exact bonds:
1-12 3-13 normalized bonds:
5-10 5-6 6-7 7-8 8-9 9-10 15-16 15-20 16-17 17-18 18-19 19-20 isolated ring systems: containing 15:

Gl:C,O

G2:O,S,N,CH3,Et,n-Pr,MeO,EtO,n-PrO

Match level: 1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:CLASS 13:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS C:\Program Files\Stnexp\Queries\rkc446h.str

chain nodes : 1 2 3 4 5 6 14 15 17 ring nodes : 7 8 9 10 11 12 chain bonds :

1-2 1-17 2-3 2-14 3-4 3-5 4-6 4-15 6-7 ring bonds :

7-12 7-8 8-9 9-10 10-11 11-12 exact/norm bonds : 1-2 1-17 2-3 3-4 3-5 4-6 6-7

exact bonds : 2-14 4-15

normalized bonds : 7-12 7-8 8-9 9-10 10-11 11-12

G2:0,S,N,CH3,Et,n-Pr,MeO,EtO,n-PrO

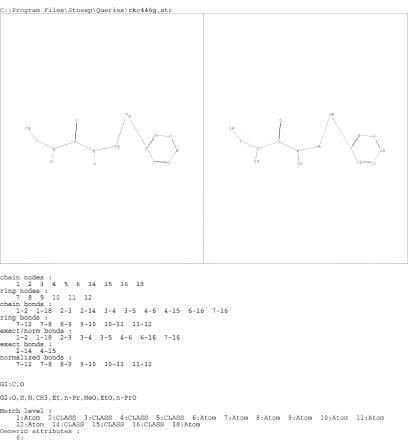
G1:C,O

Match level :

1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 14:CLASS 15:CLASS 17:Atom Generic attributes :

6: Saturation : Unsaturated

Number of Hetero Atoms : Exactly 1



Saturation

Number of Hetero Atoms : Exactly 1

: Unsaturated

C:\Program Files\Stnexp\Queries\rkc446f.str chain nodes : 10 11 12 13 14 24 25 27 ring nodes : 1 2 3 4 5 6 7 8 9 15 16 17 18 19 20 chain bonds : 6-10 10-11 10-24 11-12 11-13 12-14 12-25 14-27 15-27

isolated ring systems:
 containing 1: 15:

G1:C,O

G2:O,S,N,CH3,Et,n-Pr,MeO,EtO,n-PrO

Match level:
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 24:CLASS 25:CLASS 27:CLASS 27

1-2 1-6 2-3 3-4 3-7 4-5 4-8 5-6 7-9 8-9 15-20 15-16 16-17 17-18 18-19 19-20

3-4 3-7 4-5 4-8 6-10 7-9 8-9 10-11 10-24 11-12 11-13 12-14 12-25 14-27 15-27

1-2 1-6 2-3 5-6 15-20 15-16 16-17 17-18 18-19 19-20

14: Saturation : Unsaturated Number of Hetero Atoms : Exactly 1

ring bonds :

exact/norm bonds :

normalized bonds :

chain nodes : 10 11 12 13 14 24 25 ring nodes : 1 2 3 4 5 6 7 8 9 15 16 17 18 19 20 chain bonds : 6-10 10-11 10-24 11-12 11-13 12-14 12-25 14-15 ring bonds : 1-2 1-6 2-3 3-4 3-7 4-5 4-8 5-6 7-9 8-9 15-16 15-20 16-17 17-18 18-19 19-20 exact/norm bonds : 3-4 3-7 4-5 4-8 6-10 7-9 8-9 10-11 10-24 11-12 11-13 12-14 12-25 14-15 normalized bonds :

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isolated ring systems:
containing 1: 15:

G1:C,O

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 24:CLASS 25:CLASS

1-2 1-6 2-3 5-6 15-16 15-20 16-17 17-18 18-19 19-20

chain nodes : 10 11 12 13 14 24 25 ring nodes : 1 2 3 4 5 6 7 8 9 15 16 17 18 19 20 chain bonds : 6-10 10-11 10-24 11-12 11-13 12-14 12-25 14-15 ring bonds : 1-2 1-6 2-3 3-4 3-7 4-5 4-8 5-6 7-9 8-9 15-16 15-20 16-17 17-18 18-19 19-20 exact/norm bonds : 3-4 3-7 4-5 4-8 6-10 7-9 8-9 10-11 10-24 11-12 11-13 12-14 12-25 14-15 normalized bonds : 1-2 1-6 2-3 5-6 15-16 15-20 16-17 17-18 18-19 19-20 isolated ring systems : containing 1 : 15 : G1:C,O Match level : 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 24:CLASS 25:CLASS Generic attributes : 14: Saturation : Unsaturated Number of Carbon Atoms : less than 7 Number of Hetero Atoms : Exactly 1

C:\Program Files\Stnexp\Queries\rkc446d.str

chain nodes : 10 11 12 13 14 24 25 27 ring nodes : 1 2 3 4 5 6 7 8 9 15 16 17 18 19 20 chain bonds : 6-10 10-11 10-24 11-12 11-13 12-14 12-25 14-15 17-27 ring bonds : 1-2 1-6 2-3 3-4 3-7 4-5 4-8 5-6 7-9 8-9 15-16 15-20 16-17 17-18 18-19 19-20 exact/norm bonds : 3-4 3-7 4-5 4-8 6-10 7-9 8-9 10-11 10-24 11-12 11-13 12-14 12-25 14-15 17-27 normalized bonds : 1-2 1-6 2-3 5-6 15-16 15-20 16-17 17-18 18-19 19-20 isolated ring systems : containing 1 : 15 : G1:C,O Match level : 1.Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 24:CLASS 25:CLASS 27:CLASS Generic attributes : 14: Saturation : Unsaturated Number of Carbon Atoms : less than 7 Number of Hetero Atoms : Exactly 1

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